Effect of negative Hund's coupling in alkali-doped fullerides

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Recently, it has been well recognized that Hund,Äôs coupling (J_H) plays a crucial role in a variety of transition metal compounds. The energy scale of J_H is typically a few hundred meV. On the other hand, it has been proposed for alkali-doped fullerides (A3C60) that the energy scale of J_H is just a few ten meV, and can be dominated over the phonon-mediated exchange (Jahn-Teller type) coupling. In this situation, although the system is strongly correlated, the low-spin configuration rather than the high-spin configuration is favored, and on-site s-wave superconducting phase can emerge in the vicinity of the Mott-insulating phase (M. Capone et al., Science 296, 2364 (2002)).

To examine this scenario from first principles, we developed a method to derive a low-energy model for electron-phonon coupled systems (Y. Nomura et al., Phys. Rev. Lett. 112 027002 (2014), Phys. Rev. B 92, 245108 (2015)), and applied it to A3C60. We found that the phonon-mediated exchange coupling is as large as -50meV (favoring the low-spin configuration), while the J_H is about 30meV (favoring the high-spin configuration). We then solved the effective model by means of the dynamical mean field theory, and determined the phase diagram. The resulting phase diagram shows excellent agreement with the experiment quantitatively (Y. Nomura, et al., Sci. Adv. 1 e 1500568 (2015), J. Phys. Cond. Matt. 28, 153001 (2016)).
In the talk, I will also discuss how this unusual situation is realized with ‚Äúnegative‚Äù Hund,Äôs coupling in A3C60 but not in usual correlated materials, comparing the results for LaFeAsO.

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